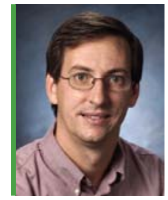
Dynamic Simulation Tools for the Analysis and Optimization of Novel Collection, Filtration, and Sample Preparation Systems



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We are developing novel multiphysics simulation tools to address design and optimization needs in the general class of problems that involve air- and water-borne species and fluid (liquid and gas phases) transport through sieving media. This new capability will be specifically designed to characterize sub-system efficiencies, such as filter efficiency, based on the details of the microstructure, surface interactions, and environmental effects.

To accomplish this, we propose to develop new lattice-Boltzmann (LB) simulation tools that will include detailed microstructure descriptions, relevant surface interactions, and temperature effects, and be able to handle both liquid and gas phase systems. We are in the process of demonstrating the applicability of this new capability to transport problems relevant to homeland security, energy, and the environment.

Project Goals

The goal of this project is to equip scientists and engineers with the computational tools to analyze and optimize novel collection, filtration, and sample preparation systems.

Relevance to LLNL Mission

This capability will be directly applicable to Laboratory programs on weapons, energy and environment, medical technology, chemical and biological counter-proliferation, genomes, and homeland security. We are developing customers in the areas of aerosol transport, adhesion and re-suspension, and fluid and chemical transport in porous media.

FY2004 Accomplishments and Results

We have continued to study particle transport in viscous fluids through complex, fibrous media. This new capability, viscousLB, includes media module and colloidal interactions. To test this, we have continued our characterization of convective transport through ordered fibrous media. Figure 1 shows that our results exhibit very good agreement with those of Reference 2. The differences are due to their use of spheres to construct their

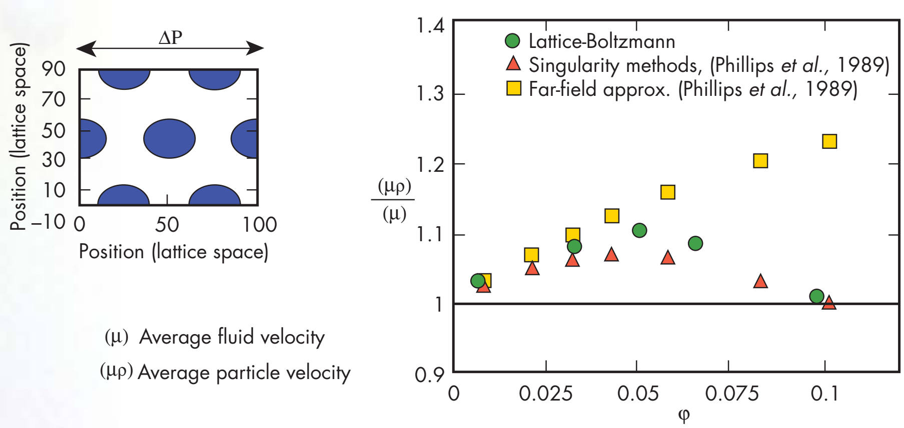

Figure 1. Comparison of convective transport coefficients predicted using the new lattice-Boltzmann capability (viscousLB) and the results of Reference 2.

cylinders, while we used cylinders directly. In addition to inclusion of the colloidal interactions module, we have expanded the capability to include Brownian forces on colloidal particles.

We have developed a gas phase fluid and particle simulation capability to enable characterization of flow and aerosol transport in complex porous media. A fourth order aerosol particle tracking routine was also developed and incorporated (Fig. 2).

To enhance the inclusion of colloidal interactions and external electric fields, we are coupling a fast multipole electromagnetic solver with viscousLB to rigorously solve the Poisson-Boltzmann equation and to include rigorous time-dependent electric fields. We are validating the aerosol transport module and the new Brownian Dynamics module, and testing the inclusion of colloidal forces in cylindrical pores for the porous membrane. Additionally, we have developed appropriate boundary conditions for gas flows, particles, and porous media. We are developing a customer base in the areas of aerosol dynamics and adhesion, flow in porous media, and flow in microenvironments with electric fields.

Related References

1. Clague, D. S., B. D. Kandhai, R. Zhang, and P. M. A. Sloot, "Hydraulic Permeability of (Un)bounded Fibrous Media Using the Lattice-Boltzmann Method," *Phys. Rev. E*, **61,** (1), pp. R1-985, 2000.
2. Phillips, R. J., W. M. Deen, and J. F. Brady, "Hindered Transport of Spherical Macro-Molecules in Fibrous Membranes and Gels," *AIChE J.*, **35,** (11), 1989.
3. Baron, P. A., and K. Willeke, Eds., Aerosol Measurement: Principles, Techniques, and Applications, Wiley Inter-Science, 2001.

FY2005 Proposed Work

Our plans are to: finalize the hybridization of the LB and Fast QR E&M capabilities and compare results with existing theory and experiment; extend our media module to incorporate filter/collector microstructures relevant to programmatic designs for a computational tool; perform analysis of filter/collector efficiencies with and without environmental temperature effects; finalize inclusion of the shear-thinning model and explore the implementation of unstructured grids to optimize physical resolution in desired domains; and apply Brownian motion capability to characterize particle petitioning and transport in nanoporous membranes, with colloidal interactions.

Factors affecting transport:
- media geometry (ordered, random)
- solid volume fraction (ϕ)
- ratio of fiber/particle size (λ)
- Knudsen number

Factors affecting surface capture:
- ratio of colloidal/aerodynamic forces
- surface charge density
- particle size

Aerosol flux calculation in an ordered filtration medium (φ = 0.05, λ = 10, Kn~0).

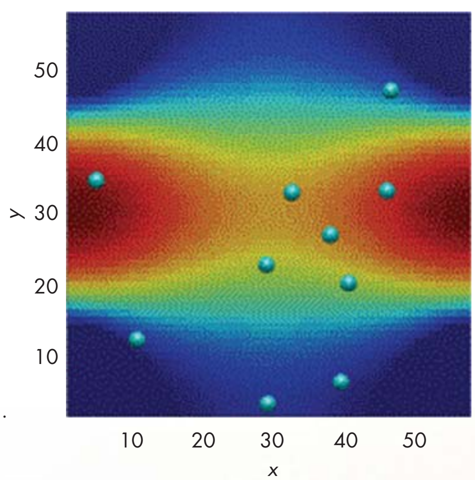

Figure 2. 2-D cross-section at a particular height of aerosol transport through a regular array of cylinders. The colors represent the magnitude of the fluid velocity. The cylinder quarters are in each corner of the periodic simulation cell.